Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:06 pm BST

PDB ID	:	5FHC
Title	:	Crystal Structure of Protective Human Antibodies 100 and 114 in Complex with Ebola Virus Fusion Glycoprotein (GP)
Authors	:	Gilman, M.S.A.; McLellan, J.S.
Deposited on	:	2015-12-21
Resolution	:	6.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

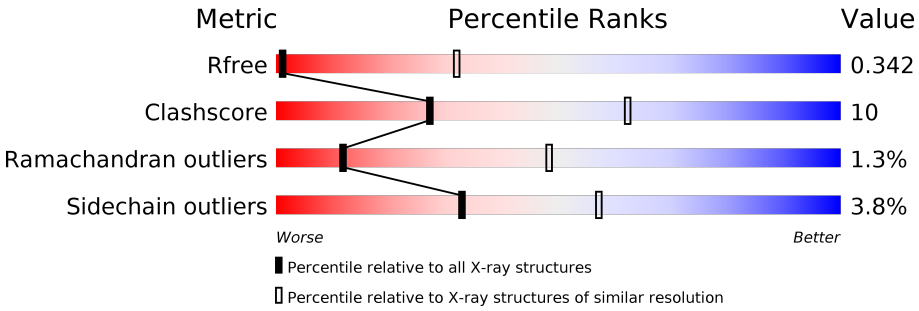
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (9.50-3.90)
Clashscore	141614	1066 (9.50-3.90)
Ramachandran outliers	138981	1000 (9.50-3.90)
Sidechain outliers	138945	1000 (9.50-3.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	J	98	70% 26%
2	K	322	45% 24% 29%
3	A	227	74% 22%
4	B	207	88% 11%
5	L	212	81% 18%
6	H	220	81% 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8854 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	98	Total	C	N	O	S	0	0	0
			747	479	130	135	3			

- Molecule 2 is a protein called Envelope glycoprotein,Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	230	Total	C	N	O	S	0	0	0
			1676	1065	287	320	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	309	SER	-	linker	UNP Q05320
K	310	ARG	-	linker	UNP Q05320

- Molecule 3 is a protein called Antibody 100 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	221	Total	C	N	O	S	0	0	0
			1667	1060	273	329	5			

- Molecule 4 is a protein called Antibody 100 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	207	Total	C	N	O	S	0	0	0
			1564	980	258	320	6			

- Molecule 5 is a protein called Antibody 114 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	211	Total	C	N	O	S	0	0	0
			1605	1004	275	321	5			

- Molecule 6 is a protein called Antibody 114 Fab heavy chain.

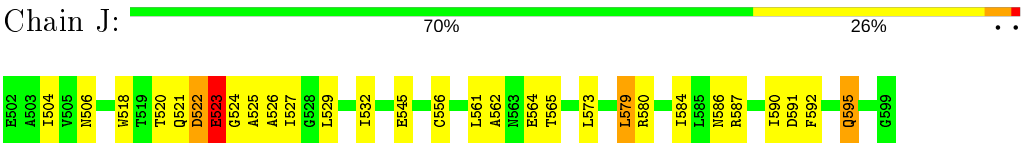
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	215	1595	1004	273	311	7	0	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

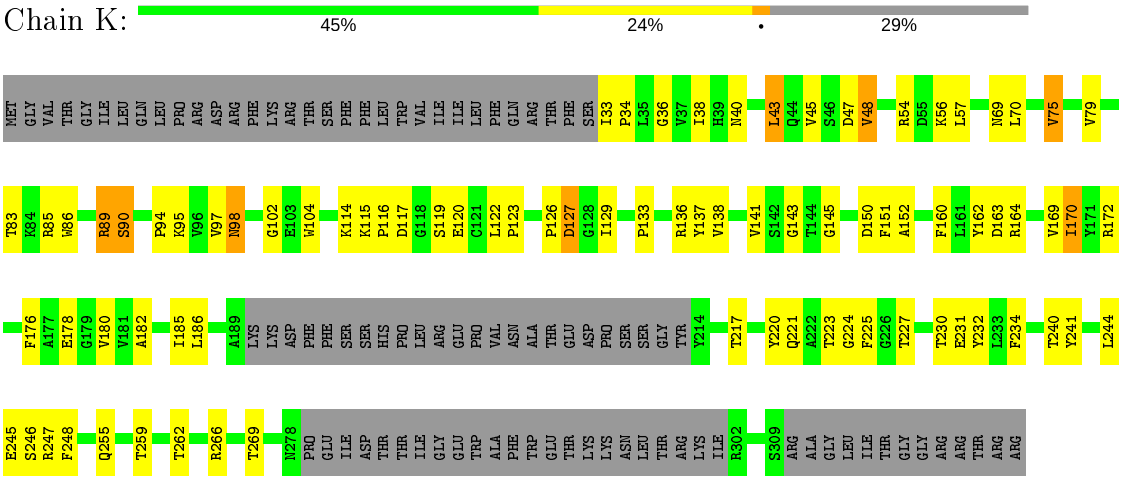
- Molecule 1: Envelope glycoprotein

Chain J:



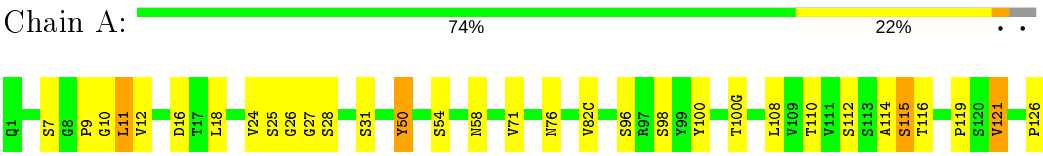
- Molecule 2: Envelope glycoprotein,Envelope glycoprotein

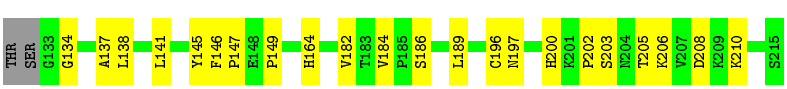
Chain K:



- Molecule 3: Antibody 100 Fab heavy chain

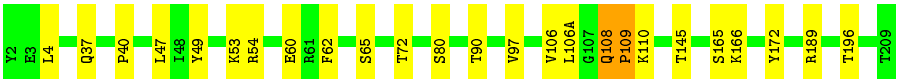
Chain A:





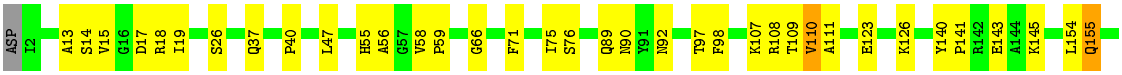
- Molecule 4: Antibody 100 Fab light chain

Chain B:



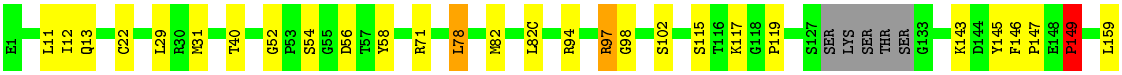
- Molecule 5: Antibody 114 Fab light chain

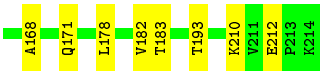
Chain L:



- Molecule 6: Antibody 114 Fab heavy chain

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	169.67Å 169.67Å 376.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.85 – 6.70 47.85 – 6.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.85-6.70) 100.0 (47.85-6.70)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 6.68Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.260 , 0.343 0.272 , 0.342	Depositor DCC
R_{free} test set	202 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	277.6	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 312.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	8854	wwPDB-VP
Average B, all atoms (Å^2)	300.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	J	0.33	0/763	0.63	0/1039
2	K	0.33	0/1712	0.58	0/2336
3	A	0.34	0/1713	0.63	0/2344
4	B	0.29	0/1603	0.53	0/2191
5	L	0.40	0/1640	0.62	0/2229
6	H	0.35	0/1629	0.64	5/2215 (0.2%)
All	All	0.34	0/9060	0.61	5/12354 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
2	K	0	1
5	L	0	2
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	149	PRO	CA-CB-CG	-7.78	89.22	104.00
6	H	149	PRO	N-CA-CB	-7.12	94.75	103.30
6	H	149	PRO	N-CD-CG	-6.86	92.90	103.20
6	H	149	PRO	CA-N-CD	-5.67	103.56	111.50
6	H	115	SER	CB-CA-C	-5.43	99.78	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	522	ASP	Peptide
2	K	54	ARG	Peptide
5	L	109	THR	Mainchain
5	L	110	VAL	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	747	0	727	32	1
2	K	1676	0	1530	72	0
3	A	1667	0	1628	36	3
4	B	1564	0	1505	15	0
5	L	1605	0	1565	31	2
6	H	1595	0	1577	33	0
All	All	8854	0	8532	176	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (176) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:11:LEU:HD13	3:A:147:PRO:HG3	1.40	1.01
5:L:108:ARG:HH12	5:L:111:ALA:HB2	1.36	0.87
3:A:11:LEU:CD1	3:A:147:PRO:HG3	2.04	0.86
5:L:108:ARG:NH1	5:L:111:ALA:HB2	1.97	0.80
5:L:155:GLN:OE1	5:L:158:ASN:ND2	2.14	0.80
3:A:10:GLY:HA2	3:A:202:PRO:HG3	1.67	0.77
6:H:210:LYS:NZ	6:H:212:GLU:OE2	2.16	0.77
2:K:223:THR:HG21	6:H:31:MET:O	1.85	0.76
4:B:40:PRO:HB3	4:B:166:LYS:HD2	1.68	0.76
3:A:200:HIS:HD1	3:A:203:SER:HG	1.34	0.75
6:H:29:LEU:O	6:H:71:ARG:NH2	2.21	0.73
3:A:108:LEU:HD23	3:A:149:PRO:HB3	1.69	0.73
3:A:112:SER:HG	3:A:146:PHE:HE2	1.37	0.72
3:A:11:LEU:HD12	3:A:110:THR:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:94:ARG:HB3	6:H:102:SER:HB2	1.73	0.71
2:K:114:LYS:NZ	5:L:92:ASN:HD21	1.88	0.71
2:K:114:LYS:HZ2	5:L:92:ASN:CG	1.95	0.70
2:K:221:GLN:HB3	6:H:97:ARG:HE	1.58	0.69
5:L:110:VAL:HG11	5:L:199:GLN:HB3	1.75	0.69
4:B:166:LYS:HG2	4:B:172:TYR:CE1	2.29	0.68
2:K:89:ARG:HG2	2:K:90:SER:N	2.08	0.68
6:H:97:ARG:NH1	6:H:97:ARG:HB3	2.10	0.67
3:A:115:SER:OG	3:A:115:SER:O	2.09	0.67
6:H:193:THR:HG23	6:H:210:LYS:HE2	1.78	0.66
1:J:562:ALA:HB1	2:K:180:VAL:HG23	1.78	0.65
1:J:527:ILE:HG22	3:A:96:SER:CB	2.28	0.64
4:B:37:GLN:HB2	4:B:47:LEU:HD11	1.78	0.64
2:K:143:GLY:HA2	6:H:98:GLY:HA2	1.80	0.64
6:H:117:LYS:N	6:H:146:PHE:O	2.31	0.64
3:A:96:SER:OG	3:A:100(G):THR:OG1	2.12	0.63
2:K:57:LEU:HD12	2:K:185:ILE:HD11	1.80	0.63
5:L:19:ILE:HD11	5:L:75:ILE:HD12	1.80	0.63
5:L:40:PRO:HB2	5:L:165:GLU:HB3	1.80	0.63
1:J:523:GLU:HB3	4:B:53:LYS:NZ	2.14	0.62
1:J:526:ALA:HB1	3:A:98:SER:CB	2.30	0.62
3:A:25:SER:O	3:A:27:GLY:N	2.34	0.59
2:K:83:THR:HG21	2:K:232:TYR:OH	2.03	0.59
1:J:504:ILE:HG23	2:K:45:VAL:HG21	1.85	0.59
1:J:526:ALA:HB1	3:A:98:SER:HB3	1.83	0.59
2:K:223:THR:HG23	6:H:97:ARG:HG3	1.85	0.58
2:K:114:LYS:HZ2	5:L:92:ASN:ND2	2.02	0.58
2:K:223:THR:CG2	6:H:97:ARG:HG3	2.34	0.58
2:K:114:LYS:NZ	5:L:92:ASN:ND2	2.51	0.57
1:J:580:ARG:NH2	2:K:127:ASP:O	2.33	0.57
6:H:149:PRO:O	6:H:149:PRO:HG2	2.04	0.57
1:J:579:LEU:HD12	1:J:579:LEU:H	1.69	0.57
2:K:231:GLU:HB2	6:H:31:MET:SD	2.45	0.56
1:J:562:ALA:HA	2:K:182:ALA:HB2	1.87	0.56
5:L:108:ARG:HG3	5:L:140:TYR:CD2	2.40	0.56
1:J:522:ASP:O	1:J:524:GLY:N	2.39	0.55
3:A:110:THR:HG21	3:A:147:PRO:HB2	1.89	0.55
2:K:162:TYR:CE1	2:K:176:PHE:HB3	2.41	0.55
2:K:227:THR:CG2	6:H:54:SER:HB3	2.36	0.55
4:B:106(A):LEU:O	4:B:108:GLN:HG2	2.07	0.54
5:L:110:VAL:HG13	5:L:141:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:595:GLN:HG3	2:K:48:VAL:HG12	1.90	0.53
2:K:117:ASP:OD2	6:H:58:TYR:HB3	2.08	0.53
2:K:126:PRO:HG2	2:K:129:ILE:HD12	1.89	0.53
6:H:97:ARG:HB3	6:H:97:ARG:HH11	1.72	0.53
1:J:504:ILE:HD11	2:K:43:LEU:HD13	1.90	0.53
1:J:561:LEU:O	1:J:565:THR:HG23	2.07	0.53
3:A:197:ASN:ND2	3:A:208:ASP:OD1	2.30	0.53
3:A:50:TYR:HE1	3:A:58:ASN:HB3	1.73	0.53
1:J:573:LEU:HD21	2:K:97:VAL:HG22	1.91	0.53
4:B:166:LYS:HG2	4:B:172:TYR:HE1	1.74	0.51
3:A:100:TYR:HE2	3:A:100(G):THR:HG22	1.76	0.51
2:K:152:ALA:HB3	2:K:170:ILE:HG13	1.93	0.51
1:J:522:ASP:O	1:J:525:ALA:N	2.43	0.51
4:B:4:LEU:HD11	4:B:90:THR:HG22	1.93	0.51
2:K:36:GLY:O	2:K:185:ILE:HG22	2.11	0.51
3:A:114:ALA:HB3	3:A:146:PHE:CD2	2.46	0.50
6:H:56:ASP:OD1	6:H:56:ASP:N	2.41	0.50
2:K:224:GLY:O	2:K:230:THR:HG22	2.12	0.50
2:K:221:GLN:HG3	2:K:241:TYR:CE2	2.47	0.50
6:H:82:MET:HB3	6:H:82(C):LEU:HD21	1.93	0.49
2:K:227:THR:HG21	6:H:54:SER:HB3	1.94	0.49
3:A:112:SER:OG	3:A:146:PHE:HE2	1.94	0.49
6:H:159:LEU:HD21	6:H:182:VAL:HG21	1.93	0.49
2:K:232:TYR:HB3	2:K:244:LEU:HD12	1.92	0.49
5:L:18:ARG:HG2	5:L:76:SER:O	2.12	0.49
2:K:255:GLN:O	2:K:259:THR:HG23	2.13	0.49
4:B:65:SER:HG	4:B:72:THR:HG1	1.61	0.49
3:A:126:PRO:HG3	3:A:138:LEU:HB3	1.93	0.48
1:J:584:ILE:O	1:J:587:ARG:HB3	2.13	0.48
2:K:221:GLN:OE1	6:H:98:GLY:HA3	2.12	0.48
2:K:114:LYS:HZ1	5:L:92:ASN:HD21	1.58	0.48
3:A:50:TYR:CE1	3:A:58:ASN:HB3	2.48	0.48
1:J:592:PHE:HA	2:K:48:VAL:HG11	1.95	0.48
4:B:40:PRO:CB	4:B:166:LYS:HD2	2.43	0.48
2:K:90:SER:HB3	2:K:150:ASP:CG	2.34	0.48
6:H:11:LEU:HB2	6:H:147:PRO:HG3	1.96	0.48
2:K:94:PRO:HB3	2:K:169:VAL:HG21	1.94	0.48
2:K:245:GLU:H	2:K:248:PHE:HE2	1.62	0.48
2:K:259:THR:HA	2:K:262:THR:HG1	1.79	0.48
2:K:259:THR:HA	2:K:262:THR:OG1	2.14	0.48
1:J:518:TRP:CZ3	2:K:133:PRO:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:595:GLN:HG3	2:K:48:VAL:CG1	2.44	0.47
1:J:518:TRP:CH2	2:K:133:PRO:HG2	2.49	0.47
2:K:115:LYS:HA	2:K:145:GLY:O	2.14	0.47
5:L:110:VAL:HG22	5:L:141:PRO:HD3	1.96	0.47
3:A:184:VAL:HG21	3:A:189:LEU:HD23	1.95	0.47
3:A:116:THR:HB	3:A:203:SER:HB3	1.97	0.47
2:K:79:VAL:HG21	2:K:220:TYR:CZ	2.49	0.47
1:J:545:GLU:HG3	2:K:104:TRP:HE1	1.79	0.47
6:H:11:LEU:HD22	6:H:147:PRO:HB3	1.97	0.46
2:K:120:GLU:HG2	2:K:172:ARG:HD3	1.97	0.46
2:K:97:VAL:HG12	2:K:98:ASN:N	2.30	0.46
3:A:100:TYR:CE2	3:A:100(G):THR:HG22	2.50	0.46
4:B:145:THR:HB	4:B:196:THR:OG1	2.16	0.46
1:J:595:GLN:HA	1:J:595:GLN:HE21	1.81	0.46
5:L:55:HIS:O	5:L:58:VAL:HG22	2.15	0.46
5:L:40:PRO:HB2	5:L:165:GLU:CB	2.45	0.46
2:K:90:SER:HB3	2:K:150:ASP:H	1.81	0.45
2:K:33:ILE:HA	2:K:34:PRO:HD2	1.76	0.45
2:K:70:LEU:HB3	2:K:75:VAL:HG21	1.97	0.45
1:J:526:ALA:HB1	3:A:98:SER:HB2	1.98	0.45
4:B:80:SER:HA	4:B:106:VAL:HG21	1.99	0.45
5:L:145:LYS:HB3	5:L:197:THR:HB	1.99	0.45
3:A:11:LEU:HD23	3:A:116:THR:HG22	1.99	0.44
2:K:97:VAL:HG12	2:K:98:ASN:H	1.82	0.44
1:J:506:ASN:HD22	1:J:556:CYS:C	2.19	0.44
2:K:85:ARG:HD2	2:K:178:GLU:OE2	2.16	0.44
2:K:123:PRO:HG3	2:K:151:PHE:CE1	2.53	0.44
2:K:141:VAL:HA	2:K:220:TYR:HB2	1.98	0.44
2:K:145:GLY:HA3	2:K:225:PHE:H	1.82	0.44
5:L:66:GLY:HA3	5:L:71:PHE:HA	1.99	0.44
2:K:231:GLU:CB	6:H:31:MET:SD	3.06	0.44
1:J:586:ASN:O	1:J:590:ILE:HG13	2.18	0.44
2:K:269:THR:O	5:L:56:ALA:HB1	2.17	0.44
3:A:12:VAL:HG11	3:A:18:LEU:HD13	1.99	0.44
6:H:119:PRO:HB3	6:H:145:TYR:HB3	2.00	0.44
5:L:14:SER:HB2	5:L:17:ASP:OD2	2.18	0.44
1:J:523:GLU:CB	4:B:53:LYS:NZ	2.81	0.43
6:H:168:ALA:HA	6:H:178:LEU:HB3	2.00	0.43
5:L:13:ALA:O	5:L:107:LYS:N	2.44	0.43
3:A:119:PRO:HB3	3:A:145:TYR:HB3	2.00	0.43
3:A:9:PRO:HB2	3:A:149:PRO:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:227:THR:HG22	6:H:54:SER:HB3	2.00	0.43
2:K:47:ASP:O	2:K:48:VAL:HB	2.18	0.43
1:J:520:THR:CG2	2:K:164:ARG:HD3	2.49	0.43
2:K:122:LEU:O	2:K:172:ARG:NH2	2.52	0.43
2:K:185:ILE:HG23	2:K:185:ILE:O	2.18	0.43
3:A:121:VAL:HA	3:A:141:LEU:O	2.19	0.43
3:A:126:PRO:HA	3:A:137:ALA:O	2.20	0.42
1:J:527:ILE:HG22	3:A:96:SER:OG	2.20	0.42
5:L:90:ASN:OD1	5:L:97:THR:HG22	2.19	0.42
3:A:24:VAL:HG13	3:A:76:ASN:ND2	2.35	0.42
4:B:109:PRO:HB2	4:B:110:LYS:H	1.67	0.42
6:H:52:GLY:O	6:H:71:ARG:HD3	2.19	0.42
3:A:134:GLY:O	3:A:186:SER:N	2.46	0.42
6:H:143:LYS:NZ	6:H:171:GLN:OE1	2.52	0.42
2:K:246:SER:O	2:K:248:PHE:N	2.53	0.42
1:J:529:LEU:HB3	1:J:532:ILE:HD12	2.02	0.42
4:B:54:ARG:HD3	4:B:62:PHE:O	2.19	0.42
1:J:573:LEU:HD21	2:K:97:VAL:CG2	2.49	0.42
6:H:22:CYS:HB3	6:H:78:LEU:HD23	2.02	0.42
2:K:241:TYR:CZ	6:H:97:ARG:NH2	2.87	0.42
5:L:13:ALA:C	5:L:107:LYS:H	2.21	0.42
5:L:123:GLU:O	5:L:126:LYS:HB2	2.20	0.42
5:L:155:GLN:CD	5:L:158:ASN:HD21	2.19	0.42
2:K:117:ASP:OD2	6:H:58:TYR:CD2	2.73	0.41
2:K:138:VAL:HB	2:K:217:THR:HG22	2.03	0.41
5:L:110:VAL:HG13	5:L:141:PRO:CD	2.50	0.41
3:A:24:VAL:O	3:A:76:ASN:ND2	2.48	0.41
5:L:89:GLN:HB2	5:L:98:PHE:CD2	2.56	0.41
2:K:160:PHE:CD2	2:K:170:ILE:HG23	2.56	0.41
2:K:38:ILE:HD11	2:K:186:LEU:HD23	2.02	0.41
3:A:206:LYS:HB2	3:A:206:LYS:HE3	1.83	0.41
6:H:12:ILE:HG13	6:H:13:GLN:N	2.35	0.41
5:L:37:GLN:HB2	5:L:47:LEU:HD11	2.02	0.41
1:J:518:TRP:CZ2	2:K:102:GLY:HA3	2.56	0.40
2:K:136:ARG:HG2	2:K:137:TYR:CE2	2.56	0.40
1:J:524:GLY:HA3	4:B:49:TYR:OH	2.21	0.40
2:K:240:THR:HG21	2:K:266:ARG:HA	2.03	0.40
5:L:141:PRO:HB2	5:L:143:GLU:OE1	2.20	0.40
5:L:58:VAL:HA	5:L:59:PRO:HD3	1.93	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:16:ASP:OD2	5:L:126:LYS:NZ[5_565]	1.70	0.50
1:J:564:GLU:OE2	3:A:54:SER:OG[2_665]	2.07	0.13
3:A:210:LYS:NZ	5:L:15:VAL:O[6_555]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	96/98 (98%)	83 (86%)	11 (12%)	2 (2%)	7 36
2	K	224/322 (70%)	183 (82%)	32 (14%)	9 (4%)	3 23
3	A	217/227 (96%)	206 (95%)	9 (4%)	2 (1%)	17 57
4	B	205/207 (99%)	196 (96%)	8 (4%)	1 (0%)	29 69
5	L	209/212 (99%)	199 (95%)	9 (4%)	1 (0%)	29 69
6	H	211/220 (96%)	205 (97%)	6 (3%)	0	100 100
All	All	1162/1286 (90%)	1072 (92%)	75 (6%)	15 (1%)	12 48

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	521	GLN
2	K	48	VAL
2	K	119	SER
2	K	163	ASP
2	K	247	ARG
3	A	26	GLY
4	B	109	PRO
2	K	56	LYS
2	K	75	VAL
3	A	115	SER
5	L	26	SER
1	J	523	GLU
2	K	40	ASN

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Mol	Chain	Res	Type
2	K	127	ASP
2	K	116	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	73/78 (94%)	69 (94%)	4 (6%)	21	47
2	K	162/278 (58%)	153 (94%)	9 (6%)	21	46
3	A	191/197 (97%)	179 (94%)	12 (6%)	18	43
4	B	178/178 (100%)	173 (97%)	5 (3%)	43	65
5	L	181/182 (100%)	179 (99%)	2 (1%)	73	84
6	H	177/182 (97%)	172 (97%)	5 (3%)	43	65
All	All	962/1095 (88%)	925 (96%)	37 (4%)	33	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	523	GLU
1	J	579	LEU
1	J	591	ASP
1	J	595	GLN
2	K	43	LEU
2	K	69	ASN
2	K	86	TRP
2	K	89	ARG
2	K	90	SER
2	K	95	LYS
2	K	98	ASN
2	K	170	ILE
2	K	234	PHE
3	A	7	SER
3	A	11	LEU
3	A	28	SER

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Mol	Chain	Res	Type
3	A	31	SER
3	A	50	TYR
3	A	71	VAL
3	A	82(C)	VAL
3	A	121	VAL
3	A	164	HIS
3	A	182	VAL
3	A	196	CYS
3	A	205	THR
4	B	60	GLU
4	B	97	VAL
4	B	108	GLN
4	B	165	SER
4	B	189	ARG
5	L	154	LEU
5	L	155	GLN
6	H	40	THR
6	H	78	LEU
6	H	97	ARG
6	H	149	PRO
6	H	183	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	512	ASN
1	J	595	GLN
3	A	1	GLN
4	B	50	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.